

**ELECTRONIC PROPERTIES OF GaAs
AND HUBBARD INTERACTION IN
TRANSITION METAL OXIDES**

By

Somalina swain

410PH2152

Under the guidance of

Prof. Biplab Ganguli



**Department Of Physics
National Institute Of Technology, Rourkela**

CERTIFICATE

This is to certify that the project thesis entitled "ELECTRONIC PROPERTIES OF GaAs & HUBBARD INTERACTION IN TRANSITION METAL OXIDE" being submitted by Somalina Swain in partial fulfillment for the requirement of the one year project course (PH592) of M.Sc. Degree in Physics of National Institute of Technology, Rourkela has been carried out under my guidance. The result incorporated in the thesis has been reproduced by using Quantum Espresso codes.

Prof. Biplab Ganguli

Dept. of Physics

ACKNOWLEDGEMENT

I would like to acknowledge my guide Prof. Biplab Ganguli for his help & guidance in the completion of my one year project & also for his encouragement. I am also very much thankful to Ph.D. research scholars of computational physics lab whose encouragement & support helped me to complete my project.

Somalina Swain

Roll no.-410PH2152

ABSTRACT

Electronic properties of GaAs semiconductor is studied using Local Density Approximation within Quantum Espresso method. GaAs is found to be a direct band gap semiconductor with band gap 1.22eV. The effect of Hubbard interaction on the absolute magnetization of FeO & MnO are also studied.

Contents

1	Introduction	2
2	Computational Technique	4
2.1	Quantum Espresso	4
2.2	Local Density Approximation	5
2.2.1	Advantage Of LDA	7
2.2.2	Disadvantage Of LDA	7
2.3	Local Density Approximation + U	8
2.3.1	Generalization Of The LDA+U functional	8
2.3.2	Application Of LDA+U	9
3	Result & Analysis	9
3.1	Electronic Properties of GaAs	9
3.2	Hubbard interaction in FeO & MnO	11
4	Conclusion	13
5	References	14

1 Introduction

Density functional theory (DFT)[1] has become the most widely used tool to study the electronic structure of atoms, molecules and solids. As it is used today, it essentially is an ingenious reformulation of the many-body problem. Instead of trying to solve the Schroedinger equation of interacting electrons directly, the problem is cast in a way such as to make it tractable in an approximate, but in many cases surprisingly accurate way. The success of DFT is largely due to the availability of increasingly accurate approximations to the central quantity of DFT, the so-called exchange-correlation energy functional.

While the simple local density approximation (LDA) proved to be surprisingly accurate especially in solid state physics, only the advent of the so-called generalized gradient approximations (GGAs) with their increased accuracy led to an explosion of applications of DFT in quantum chemistry[1].

The development of new, improved functionals is an ongoing effort. In this contribution we are dealing with a particular class of approximations which are explicit functionals of the Kohn-Sham orbitals rather than explicit functionals of the density (such as LDA or GGA). Treatment of orbital functionals in the DFT framework requires the use of the so called optimized effective potential (OEP) method to compute the corresponding effective single-particle

potentials[1].

Due to the simplification in their exchange correlation functional form & other unphysical features like self-interactions, LDA & GGA fail to describe the system with strong coulomb interactions such as transition metal oxides & rare earth compounds[2].

2 Computational Technique

2.1 Quantum Espresso

Quantum Espresso is a variety of numerical methods & algorithms aimed at a chemically realistic modeling of materials from the nanoscale upwards, based on the solution of the density functional theory(DFT).

It is an integrated suite of computer codes for electronic structure calculations and materials modeling based on DFT, plane waves and pseudopotentials(norm conserving, ultrasoft and projector augmented wave) to represent the electron-ion interactions[4].

The ESPRESSO stands for opEn Source Package for Research in Electronic Structure, Simulation & Optimization. The codes are constructed around the use of periodic boundary conditions, which allows for a straightforward treatment of infinite crystalline systems [4].

Quantum espresso can do the following basic computations[4].

1. Calculation of the Kohn-Sham(KS) orbitals and energies for isolated systems, and of their ground state energies.
2. Complete structural optimizations of the microscopic(atomic coordinates) & macroscopic degrees of freedom.
3. Ground state of magnetic or spin polarized systems.

4. Spin orbit coupling & non-collinear magnetism.
5. Ab-initio molecular dynamics(MD) in a variety of thermodynamical ensembles.
6. Density functional perturbation theory(DFPT),to calculate second and third derivatives of the total energy at any arbitrary wavelength.
7. Calculation of phonon dispersion, nudged elastic band.

For our electronic structure calculation we used the Quantum Espresso existing code. Electron corrections are taken into account within the local density approximation(LDA) & plus advanced functionals like Hubbard U corrections (LDA+U). Many different exchange-correlation functionals are available in the frame work of the LDA or generalized gradient approximations(GGA) plus advanced functionals like Hubbard U corrections. The latter is an area of very active development & more details is based on hybrid functionals & related Fock exchange techniques[2].

2.2 Local Density Approximation

Local Density Approximation are a class of approximations to the exchange-correlation (XC) energy functional in density functional theory (DFT) that

depend solely upon the value of the electronic density at each point in space (and not, for example, derivatives of the density or the Kohn-Sham orbitals). Many approaches can yield local approximations to the XC energy[6].

However, overwhelmingly successful local approximations are those that have been derived from the homogeneous electron gas (HEG) model. In this regard, LDA is generally synonymous with functionals based on the HEG molecules, which are then applied to realistic molecules [6].

In general, for a spin-unpolarized system, a local-density approximation for the exchange-correlation energy is written as,

$$E_{xc}^{LDA}[\rho] = \int \rho(r) \epsilon_{xc}(\rho) dr \quad (1)$$

Where ρ is the electron density & ϵ_{xc} the exchange-correlation energy density, is a function of the density alone. The exchange-correlation energy is decomposed into exchange and correlation terms linearly[6].

$$E_{xc} = E_x + E_c \quad (2)$$

so that separate expressions for E_x & E_c are sought. The exchange term takes on a simple analytic form for the HEG. Only limiting expressions for the correlation density are known exactly, leading to numerous different approximations for ϵ_c .

Local Density Approximation are important in the construction of more sophisticated approximations to the exchange-correlation energy, such as gener-

alized gradient approximations or hybrid functionals, as a desirable property of any approximate exchange-correlation functional is that it reproduce the exact results of the HEG for non-varying densities. As such, LDA's are often an explicit component of such functionals.

2.2.1 Advantage Of LDA

1. It works well in cases of energetics matter.
2. Errors in the approximation E_x & E_c cancels each other.
3. LDA satisfied the rule for the exchange correlation hole.

2.2.2 Disadvantage Of LDA

1. Poor eigenvalues.
2. Lack of derivative discontinuity at integer.
3. Gaps too small or no gap.
4. Spin & orbital momentum is too small.
5. For transition metal oxides it fails.
6. When it deals with excited state properties it fails.
7. Self interaction problems.

8. Mirror image charges.
9. Two body correlations.

2.3 Local Density Approximation + U

Then we use LDA+U method for advanced result.i.e.Hubbard U correction. LDA+U can be considered as one of the most efficient approaches as it is successful in understanding strongly correlated systems due to the on-site Coulomb correlation effect & the modest computational time. It requires same computational cost as LDA because of the local correction in real space [6].

It is also due to for unrestricted Hartee-Fock treatments for the localized orbital states.

2.3.1 Generalization Of The LDA+U functional

It can be generalized in the following issues [7].

1. Rotational invariant formulation of the LDA+U functional.
2. LDA average of the on-site coulomb interactions.
3. Choice of the basis,a construction of the local projection operator.
4. Self -consistent determination of the parameters.

2.3.2 Application Of LDA+U

1. It is applied for the study of Oxide engineering.
2. For Ultra small electronic devices.
3. Large scale electronic structure is calculated.
4. Also applied with the local pseudo atomic orbital basis.
5. Also applied to Quantum phase transitions in the following cases[7].
 - (a) Metal-Insulator transitions.
 - (b) Quantum critical point.
 - (c) Spin/orbital/charge ordering phenomena.

3 Result & Analysis

3.1 Electronic Properties of GaAs

GaAs has equal number of Ga & As ions distributed on the diamond lattice so that each has four of the opposite kind as nearest neighbors. It is a face centered cubic lattice with two point basis. It has a higher saturated electron velocity and higher electron mobility, allowing gallium arsenide transistors to function at frequencies in excess of 250 GHz. It is a III/V semiconductor, and is used in the manufacture of devices such as microwave frequency

integrated circuits, monolithic microwave integrated circuits, infrared light-emitting diodes, laser diodes, solar cells and optical windows[8] .

From Fig.1 we found the kinetic energy cutoff 25Ry for infinite plane wave

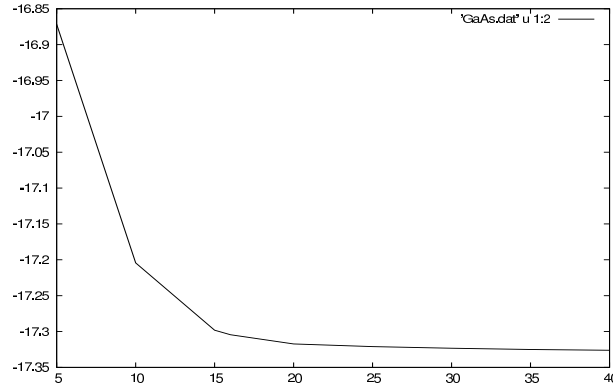


Figure 1: Kinetic energy cutoff of GaAs

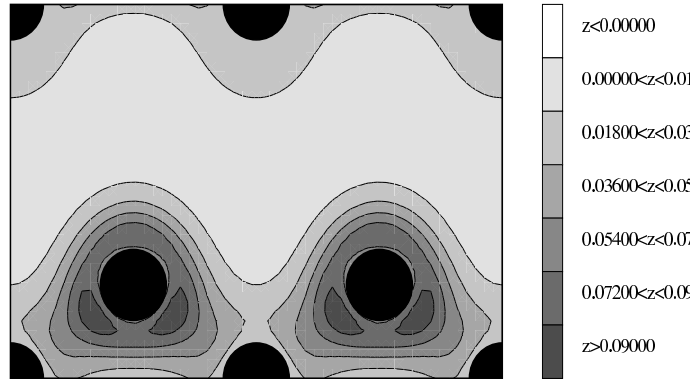


Figure 2: Charge density plot of GaAs

basis set. From Fig.2 it is found that the GaAs is covalently bonded. From figure 3, the band structure is calculated to be 1.22eV for GaAs which is in good agreement with experimental result [8]. The band structure of GaAs was calculated using empirical pseudopotential method(EPM) with Quan-

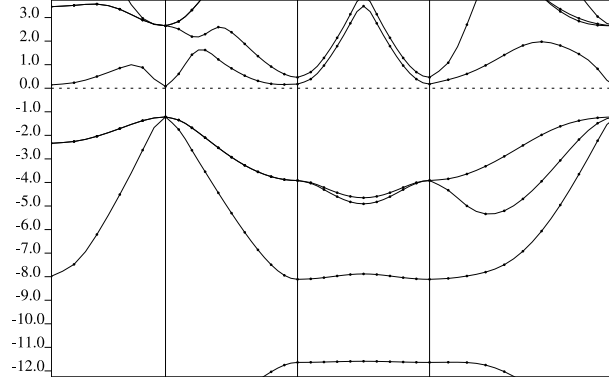


Figure 3: Band structure plot of GaAs

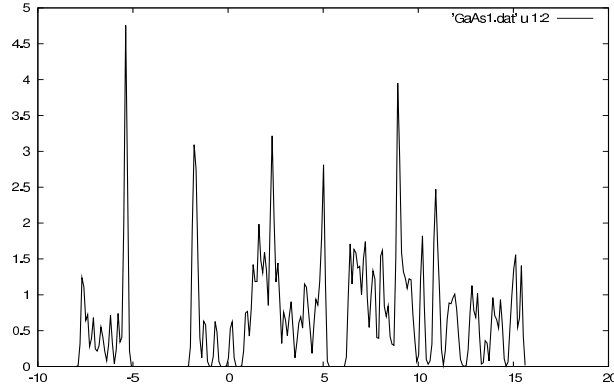


Figure 4: Density of state (DOS) of GaAs

tum Espresso existing code.

3.2 Hubbard interaction in FeO & MnO

These are transition metal oxides. It is one of the most interesting classes in solids. These are the examples of strongly correlated electron systems. It has core level binding energies. Spin orbit splittings & exchange splittings are found to exhibit interesting variations with the oxidation state of the metal & nuclear charge. It is used for the study of satellite structure, final state

effects in x-ray photo spectra ,catalytic activity & semi-conductive properties [9].

For FeO,

The absolute magnetization of FeO using local density approximation is found to be 7.09 Bohr mag/cell. When the hubbard energy of 0.31Ry is applied then the absolute magnetization is enhanced to 7.25 Bohr mag/cell.

For MnO,

Using LDA we get absolved magnetization is 9.42 mag/cell but with the addition of Hubbard interaction energy 0.08Ry, the absolute magnetization is increased to 9.50 Bohr mag/cell.

4 Conclusion

The electronic properties like band structure, density of states and charge density of GaAs are studied using quantum espresso code. The band gap is found to be 1.22 eV. The study of interaction of Hubbard potential in FeO and MnO shows the enhancement of absolute magnetization.

5 References

1. NIC Series, Vol. 31, ISBN 3-00-017350-1, pp. 299-334, 2006.
2. www.scielo.br/scielo.php.
3. Myung Joon Han et.al., Phys. Rev. B 73, 045110 (2006).
4. P.Giannozzi et.al., J.Phys.:Condens. Matter 21(2009) 395502(19pp).
5. S.Mishra,B.Ganguli, Solid State Commun.151(2011) 523-528.
6. W.N.Honeyman, K.H. Wilkinson,J.Phys.D:Appl.Phys.4(1971)1182.
7. Jaejun Yu,school of Physics, Seoul National University, 2nd KIAS workshop, 2005/06/13.
8. J.R.Chelikowsky and M.L.Cohen, Phys. Rev. Let. 32, 674-677 (1974).
9. www.jstor.org.